1,4-Dioxin, 2,3-dihydro-

Other names: p-Dioxin, 2,3-dihydro-
Inchi: InChI=1S/C4H6O2/c1-2-6-4-3-5-1/h1-2H,3-4H2
InchiKey: HIZVCIIORGCREW-UHFFFAOYSA-N
Formula: C4H6O2
SMILES: C1=COCCO1
Mol. weight [g/mol]: 86.09
CAS: 543-75-9

Physical Properties

Property code	Value	Unit	Source
affp	823.50	kJ/mol	NIST Webbook
basg	792.80	kJ/mol	NIST Webbook
gf	-127.32	kJ/mol	Joback Method
hf	-257.45	kJ/mol	Joback Method
hfus	14.06	kJ/mol	Joback Method
hvap	34.55	kJ/mol	Joback Method
ie	8.07 ± 0.02	eV	NIST Webbook
log10ws	-0.41		Crippen Method
logp	0.504		Crippen Method
mcvol	63.800	ml/mol	McGowan Method
pc	5519.63	kPa	Joback Method
tb	367.30	K	NIST Webbook
tc	579.93	K	Joback Method
tf	200.36	K	Joback Method
vc	0.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	107.10	J/mol×K	368.20	Joback Method
cpg	150.26	J/mol×K	544.64	Joback Method
cpg	142.64	J/mol×K	509.35	Joback Method
cpg	134.53	J/mol×K	474.07	Joback Method
cpg	125.91	J/mol×K	438.78	Joback Method

cpg	116.78	J/mol×K	403.49	Joback Method
cpg	157.40	J/mol×K	579.93	Joback Method
dvisc	0.0004081	Pa×s	368.20	Joback Method
dvisc	0.0005599	Pa×s	340.23	Joback Method
dvisc	0.0008132	Pa×s	312.25	Joback Method
dvisc	0.0012709	Pa×s	284.28	Joback Method
dvisc	0.0021897	Pa×s	256.31	Joback Method
dvisc	0.0043106	Pa×s	228.33	Joback Method
dvisc	0.0102525	Pa×s	200.36	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C543759&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume